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Simulation method of the low-Re flows in the packed bed technological equipment

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Abstract. The paper shows the semiempirical method of a numerical simulation of the low-Re flows in the packed bed technological apparatus. The proposed method is based on the Navier-Stokes equations modification by the linear momentum sources equations in the packed bed zones. It is found that the simulation error of the proposed method is not more than 6.2% for low-density finite element meshes. The average value of the simulation error is about 3.0% for all shown cases. It was found that the proposed method simulation error almost independent on the mesh density. In the main, the simulation error is determined by the linear momentum sources equations approximation error.

1. Introduction

Packed bed columns are widely used in the chemical industry. Many technological processes like a sorption, a chemisorption, an ion exchange, catalytic chemical reactions proceed on the contact surfaces of the packed bed particles and the technological gases and liquids flow. Moreover, many hydromechanical and hydrodynamical processes (like processes in filters, shaft furnace processes, gas-solid and liquid-solid metallurgical and concentration processes) are determined by the hydrodynamics of the low-Re flows in pores of packed particles.

Classical engineering calculation of the packed bed equipment hydrodynamics consists of the pressure drop calculation in the packed bed layer. Most often the packed bed hydraulic resistance may be calculated as a sum of drops due to friction and kinetic losses by Ergun's equation [1]:

$$\frac{\Delta p}{L} = \frac{150\mu(1-\xi)^2}{d_p^2 \xi^2} u_{eff} + \frac{1.75\rho(1-\xi)}{d_p \xi^3} u_{eff}^2, \quad (1)$$

or in the case of low-Re (laminar) flow:

$$\frac{\Delta p}{L} = \frac{150\mu(1-\xi)^2}{d_p^2 \xi^2} u_{eff}. \quad (2)$$

There Δp is the pressure drop, Pa; L is the packed bed layer height, m; μ is the liquid viscosity, Pa·s; ξ is the packed bed porosity; d_p is the packed bed particle size (diameter), m; u_{eff} is the fluid effective velocity, m/s; ρ is liquid density, kg/m³.

In cases of the solid particle's irregular or complex shape, the packed bed variable porosity and for the other special cases Ergun's equation may be modified [2, 3, 4, 5, 6, 7]. Idelchik shows Ergun's equation in the dimensionless form [8]:



$$\Delta p = \lambda \frac{L}{d_p} \frac{\rho u_{eff}^2}{2} = \left(\frac{A}{Re} + B \right) \frac{L}{d_p} \frac{\rho u_{eff}^2}{2}, \quad (3)$$

$$Re = \frac{u_{eff} d_p \rho}{\mu}. \quad (4)$$

There Re is the Reynolds number calculated from effective velocity and solid particle size; λ is effective friction coefficient; A and B are empirical coefficients depended on the particle form, the particle surface shape, and the packed bed porosity.

The calculation error of the Ergun's equation-based methods is about 20-30% for the low-Re flows [8]. The accuracy of these methods is enough for the estimated engineering calculations but may be insufficient for the design calculations.

CFD codes use many methods of the pressure drop simulation in a packed bed. There are Darcy's low-based models [9, 10], various porous media models [10, 11], modified Ergun's methods, and another pressure drop coefficients models. All of them can be summarized as:

$$S_i = C_1 \mu u + C_2 \rho u^2. \quad (5)$$

There S_i is the momentum source along the coordinate axis, N/m^3 (Pa/m); C_1 and C_2 are the coefficients depend on the particles size and shape, the packed bed porosity and the flow velocity; u is the flow velocity along the coordinate axis, m/s . Frequently the coefficients C_1 and C_2 vary no-linear with flow velocity change. Moreover, often for the low-Re flows the coefficients C_1 and C_2 take large values. Thus, the mathematical errors of the small and large numbers manipulations (floating-point errors) may occur. These errors often lead to the solution stability decreasing or the solver crashing.

This paper proposes the stable semiempirical CFD simulation method of the low-Re flows in the packed bed equipment.

2. Experimental research

Figures 1 and 2 show the scheme and the photo of the experimental test-stand respectively. The experimental test-stand consists of the packed column 1, the filters 2, the inlet chamber 3, the outlet chamber 4, the control valve 5, the flexible pipelines 6, the differential manometer PD , and the flow meter F .

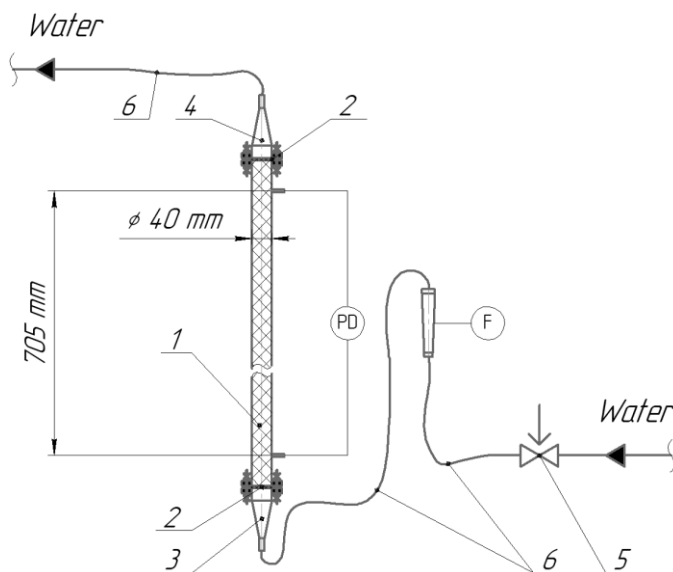


Figure 1. Scheme of the experimental test-stand: 1 – packed column, 2 – filters, 3 – inlet chamber, 4 – outlet chamber, 5 – control valve, 6 – flexible pipelines, PD – differential manometer, F – flow meter.



Figure 2. Photo of the experimental test-stand.

The water from the plumbing enters the flexible pipelines 6, passes the control valve 5 and flow meter F , enters the inlet chamber 3, fills the packed column 1, and exits from the outlet chamber 4 through the flexible pipeline 6 to the sewerage. The packed column 1 is the cylindrical vessel made from transparent PLA. The internal diameter of the column is 40 mm. The column filled with the granular particles. The average diameter of the particles is about 0.8 mm. The porosity of the packet bed is 0.45. At the top and at the bottom of the column 1 there are filters 2 with the cell size 0.5 mm. The filters 2 prevent the losses of the granular particles from the column 1.

The water flow is controlled by the control valve 6 and measured by the flow meter F . The hydraulic resistance of the packed bed is measured by the differential manometer PD . The connection fittings of the differential manometers are located at the distance of 100 mm from the filters. The distance between the connection fittings is 705 mm.

The water flow varies in the range of 30-70 l/h. The result of the experimental measurements is the dependence of the packed bed hydraulic resistance on the water flow through the column.

3. Experiment results and discussion

Figure 3 shows the measured and calculated by the equation (1) dependencies of the packed bed column hydraulic resistance on the effective water velocity in the packed column. Figure 4 shows the dependencies of the effective friction coefficient calculated from equation (1) and by the measurement results processing on the Re number. For the packed bed hydraulic resistance and the effective friction coefficient calculation's equation (1) was supplemented with the hydrostatic pressure terms.

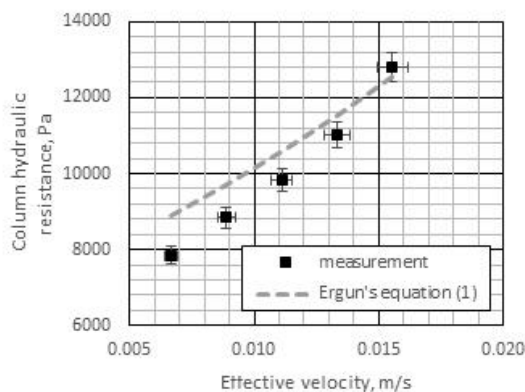


Figure 3. Dependencies of the measured and calculated column hydraulic resistance on the effective water velocity in the packed column.

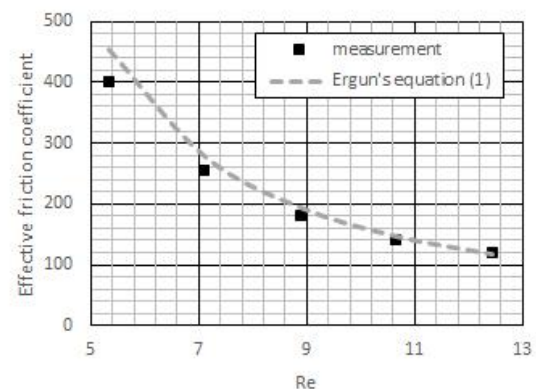


Figure 4. Dependencies of the measured and calculated effective friction coefficient on the Reynolds number.

Figure 3 shows, that the packed bed column hydraulic resistance depends on the effective velocity to the second degree. Therefore, for the effective velocities in the range of 0.007-0.016 m/s, the packed bed hydraulic resistance depends on the frictional and kinetic losses both. Thus, it is unacceptable to ignore the second term in the right part of the equation (1) in our case. The maximum and the average calculation error by equation (1) are 13.4% and 7.5% respectively. The experimental measurement errors of the hydraulic resistance and the water flow measurement by Student's method [12] are 3.0% and 4.4% respectively. The experimental packed bed hydraulic resistance rises faster than calculated packed bed hydraulic resistance with effective velocity growth.

Figure 4 shows, that the effective friction coefficient decreases nonlinearly with increasing the Reynolds number. For the Reynolds number in the range of 5-12, the measured and calculated effective friction coefficients are reduced by 68% and 74% respectively. The nature of the shown change of the effective friction coefficient with the Reynolds number rising corresponds well to the reference Information [8].

4. Numerical simulation

The mathematical model based on a steady-state isothermal Navier-Stokes momentum conservation equation with the additional momentum source term. For steady-state isothermal conditions, Navier-Stokes momentum conservation equation takes form [13]:

$$(\rho u_j) \frac{\partial u_i}{\partial x_j} = \frac{dp}{dx_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \right] + \rho g_i + S_i. \quad (6)$$

There ρ is the density, kg/m³; u is the velocity, m/s; i, j are the indexes of the longitudinal and the transverse directions of the flow; x is the coordinate, m; p is the pressure, Pa; μ is the viscosity, Pa·s; δ_{ij} is the metric tensor; g is the gravity force acceleration, m/s²; There S_i is the momentum source along the coordinate axis, N/m³ (Pa/m). It should be noted that the momentum source dimension coincides with the Ergun's equation (1) dimension.

It was shown earlier that the hydraulic resistance of the packed bed increases nonlinearly with increasing the effective velocity. Moreover, the value of the effective velocity is of the order 10⁻³, and the value of the effective friction coefficient is of the order 10². In that the effective velocity enters the equation (1) in the second degree, it is difficult to use Ergun's equation original form for the CFD simulation due to the risk of the solver crashing cause of the floating-point error.

To solve this problem, we used the approach from our earlier work [14]. In our work [14] we propose to approximate the experimental dependence of the packed bed hydraulic resistance on the effective velocity by the sequence of the linear equations. In the previous work [14] we used effective velocity order coefficients to prevent the floating-point error. This approach allows us to rise the solution stability, but it has no physical sense. Moreover, we need to reprocess experimental data approximation in case of the fluid density or viscosity changes with this approach. The importance of this remark increases significantly in the case of a change in temperature or chemical composition of the fluid in the packed bed. Thus, we propose to use the sequence of linear approximations of the dependences of the packed bed specific hydraulic resistance on the Reynolds number. This will allow us to consider the fluid rheological properties and to rise the approximating linear equations argument order with the physical sense retention.

Thus, the momentum source equation for the packed bed zones takes form:

$$S_i = A \cdot Re + B. \quad (7)$$

There A and B are the approximation coefficients depended on the Reynolds number. The scheme of the experimental data approximation and the values of the approximation coefficients for our case are shown on the figure 5 and in the table 1 respectively. It is very important to note that for the first from-zero experimental data section the value of the linear approximation equation must be equal zero in the Re zero point. Otherwise, the packed bed will generate a negative momentum at zero flow velocity, and the solution instability or the solver crashing may occur.

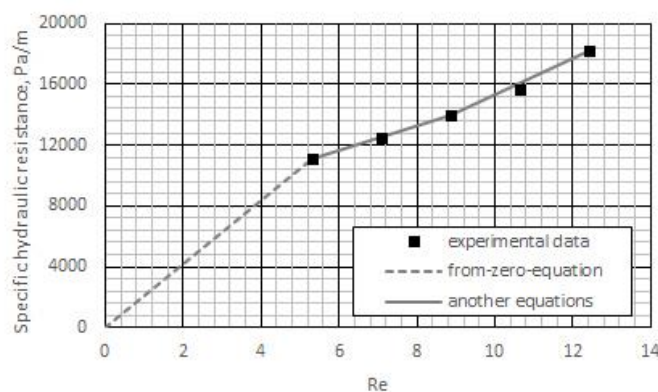


Figure 5. Scheme of the experimental data approximation: the from-zero-equation interval is indicated by the dashed line since there is no experimental data for this interval.

Table 1. Approximation equations coefficients

Re interval	A	B	Approximation error, %
0 – 5.3	2088	0	0.01
5.3 – 7.9	795	6888	0.02
7.9 – 12.4	1192	3361	2.75

5. Simulation results and discussion

Figure 6 shows the measured, calculated by Ergun's equation (1) and CFD simulated dependencies of the packed bed column hydraulic resistance on the effective water velocity in the column. For CFD simulation we used ANSYS Fluent code with the additional momentum source compiled user-defined function (UDF). The calculation was carried out for the 2D axisymmetric geometry with three triangular meshes of 31550, 7792 and 1152 elements densities. The element sizes for these meshes were 1, 2 and 5 mm respectively. Simulated results for all cases are almost equal. Table 2 shows the simulated hydraulic resistance values.

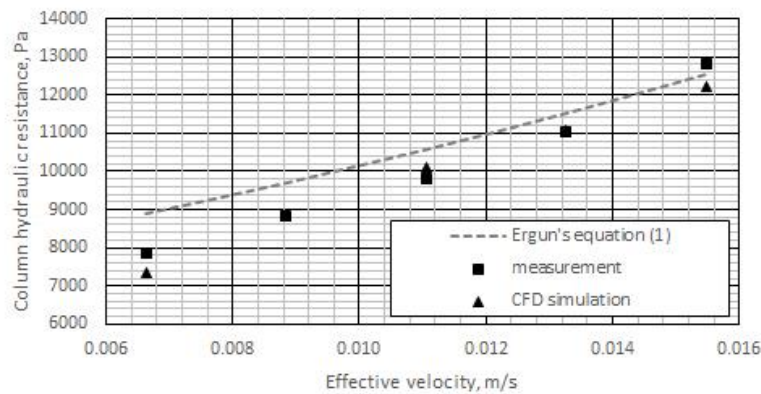


Figure 6. Dependencies of the measured, calculated and CFD simulated packed bed column hydraulic resistance on the effective water velocity in the packed column.

Table 2. Packed column CFD simulated hydraulic resistance

Effective velocity, m/s	Measured hydraulic resistance, Pa	Simulated hydraulic resistance, Pa		
		31550 elements mesh	7792 elements mesh	1152 elements mesh
0.007	7840	7353	7359	7351
0.009	8835	8828	8841	8832
0.011	9829	10093	10105	10090
0.013	11019	11100	11117	11104
0.015	12813	12233	12129	12114

The maximum and the average CFD simulation error for all meshes are 6.2% and 3.0% respectively. Thus, the error of the proposed CFD simulation method is less than Ergun's equation (1) calculation error on 52-56%. Besides, the error of the proposed simulation method is almost independent of the mesh density for considered element sizes. The discrepancy of simulation results for considered meshes is about 5-20 Pa (0.2 %). The maximum errors for all simulation cases are in the same values of the effective velocities. Thus, we suppose that the simulation error depends on the experimental data approximation error for the most part.

It should be noted that all simulations were stable, but there was not the solution convergence in all cases due to meshes low density. Thus, the proposed simulation method of the low-Re flows in the packed bed may be used for the technological equipment CFD simulation.

6. Conclusion

We proposed the simulation method of the low-Re flows in the packed bed technological equipment. The proposed method is based on the Navier-Stokes momentum conservation equation modification using the linear approximations of the specific hydraulic resistance dependences on the Reynolds number sources. The proposed method considers the changes in the fluid rheological properties in the packed bed and rises the solution stability. It is shown that the average simulation error of the proposed method is about 3.0% for the considered packed particles and Reynolds number interval. The average calculation error of Ergun's equation is about 7.5% for the same conditions. Thus, the proposed simulation method may be used for technological equipment research and design.

It is shown that the error of the proposed simulation method almost independent of mesh density. Apparently, the error of the proposed method depends on the experimental data approximation error for the most part. Thus, the proposed method may be used for low calculating power CFD simulation.

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